

1-Methyl-6-(2-methylphenyl)-1,6-dihydro-3-pyridinecarbonitrile  
27531-42-6 | DTXSID60299776

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 7.47

Global applicability domain: Inside

Local applicability domain index: 5.14e-01

Confidence level: 5.72e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Thiram</div> <div>Measured: 3.39</div> <div>Predicted: 3.91</div>	<div>Image not found</div> <div>Isophorone</div> <div>Measured: 2.00</div> <div>Predicted: 3.19</div>	<div>Image not found</div> <div>2-(Thiocyanomethylthio)benzothiazole</div> <div>Measured: 209</div> <div>Predicted: 13.0</div>
<div>Image not found</div> <div>Triallylamine</div> <div>Measured: 3.55</div> <div>Predicted: 4.23</div>	<div>Image not found</div> <div>O,O-Diethyl dithiophosphate</div> <div>Measured: 5.01</div> <div>Predicted: 5.43</div>	